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Resonant double electron capture by fast He^{2+} from helium: the first-order Born approximation with correct boundary condition

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Abstract. The first-order Born approximation with correct boundary condition is applied in a study of the resonant double electron capture by fast He^{2+} from helium. A configuration-interaction wave function is employed to describe the ground state of helium. Total cross section as a function of the impact energy is calculated and compared with experimental and theoretical values.

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Introduction

The double electron capture in high energy $He^{2+} + He$ collision has received considerable interest from both theoretical and experimental points of view over the past decades. The first experimental studies were performed several years ago [1–3]. Comparing these earlier results to the new ones [4, 5] some deviation could be found in the energy dependence of the total cross section data in the impact energy range 0.4–6.0 MeV [6] (see Fig. 2 below). The data from [1, 5] are smooth continuation of each other while the results from [2, 3] exhibit different qualitative dependence. At lower energies the data of DuBois [4] confirm the tendency predicted by the measurement of Pivovar et al. [2]. The newest experimental results of Schuch et al. [7] agree with the data of de Castro Farina et al. [5] at 1.5 MeV impact energy, however their experimental total cross section values are somewhat lower than it could be predicted from [5] at the highest energies.

The theoretical studies for the above mentioned reaction are concentrated mainly on the impact energy range 0.4–1.5 MeV, where most of the experimental data are available. The calculation of Gerasimenko [8] based on a first Born like calculation seems to overestimate the experimental data. The two-state atomic expansion of Theisen and McGuire [9] is in good agreement with the experimental data at lower energies, however it seems to overerstimate the process at high collision energies. As a higher-order perturbation approach the Continuum Distorted Wave (CDW) approximation was given by Gayet et al. [10]. Two different types of wave functions (hydrogenic and Hartree Fock (HF)) were applied for representing the final state. The difference between the two cases reveals that the two-electron capture is very sensitive to the choice of the orbitals formed around the projectile. In a further study [6] the Continuum Distorted Wave Eikonal Initial States approximation (CDW-EIS) was applied, too, and a very good agreement with group of experiments [1, 5] was found in the studied energy range 0.2–3.0 MeV [6].

All the theoretical descriptions mentioned above are based on the independent particle (IPA) approximations [11, 12]. Namely, the interelectron Coulomb interaction is approximated by an appropriate average field, such as the Hartree-Fock atomic model potential. So the IPA completely ignore both the 'dynamic' (effect of the electron-electron interaction in the scattering region) and 'static' (effect of the electron-electron interaction in the ground states) correlations. Consequently, in this formalism the double capture transition probability P leads to the product $P_1 P_2$, where P_1 and P_2 are the probabilities for the first and second capture events, respectively.

Recently attempts have been made to avoid the IPA through the appropriate description of the correlated electronic orbitals of the unperturbed hamiltonians. Crothers and McCarroll [11] used the Pluvinage wave function to describe the initial state applying the so-called continuum-continuum correlation within the CDW approach. The single differential cross section (SDCS) values are lower than those of Gayet et al. [6, 10] applying a similar CDW model in the framework of the independent particle approach. Deco et al. [13] used the configuration-interaction (CI) wave function for describing the initial and final states also in the frame of the CDW approach. The SDCS values, which are higher than the corresponding ones of Gayet et al. [10] (with HF orbitals, see [13]) especially at higher energies, demonstrates the role of the static correlation in the de-

scription. More recently Gravielle et al. [14] calculated the double electron capture process in the frame of the second-order distorted wave formalism. The electronic repulsion was also included in first order as a perturbation potential during the collision in their calculation, and the SDCS values were very similar to the ones of Crothers et al. [11]. Moreover, a negligible difference was found between the results using HF and CI wave functions. As it is seen, the static correlation has a different contribution in the different theoretical models used for describing the double capture in $He^{2+}+He$ collision (e.g. the differences between the results using uncorrelated and correlated wave functions is and is not negligible in the study [13] and [14], respectively). However, these deviations does not change the results significantly and the experimental values with similar or larger deviations is not able answer the question regarding the role of the static correlation in description of these reaction. It is interesting to note that all of these models still use the product or the sum of the products of one electron capture amplitudes, which correspond to the participating individual orbitals in a correlated wave function.

All of the experimental data mentioned refer to the capture into all states of the helium, in contradiction with the theoretical SDCS values referring to the resonant double capture, i.e.:

$$He^{2+}+He(1s^2)\rightarrow He(1s^2)+He^{2+}. \tag{1}$$

Gravielle et al. [14] found that the contribution from capture into excited states is about 30% of the cross section for capture into the ground state at 180 keV. This contribution decreases with increasing impact velocity and so it is not likely to affect the behavior of the SDCS as a function of the impact energy.

The aim of the present work is to study the process (1) in the frame of the first Born approximation with correct boundary conditions (*B1B*) [15]. Recently the *B1B* model has been satisfactory used for the description of single electron capture phenomena. It gives comparable values to the ones of higher order models (CDW and CDW-EIS) at not too high impact velocities where the Thomas scattering is negligible [15–17]. So the present study try also to find an answer to the question whether a similar conclusion could be valid in describing the double capture process (1). In the present calculation the bound states are described by CI wave function.

In the next section we give the details of our derivation and the last section contains comparison of the present results with experimental and other theoretical values.

Unless stated otherwise atomic units will be used throughout.

Theory

Consider the following two-electron capture process

$$Z_P+(Z_T,e_1,e_2)_i\rightarrow(Z_P,e_1,e_2)_f+Z_T, \tag{2}$$

where Z_K ($K=P$, T) is the charge of the Kth nucleus and e_k ($k=1,2$) is the kth electron. The parenthesis $(..)_j$ symbolizes the bound states characterized by the $j(=i, f)$ quantum numbers. Let $\mathbf{r}_{Kk}$ be the position vectors of the kth electron relative to the Kth nucleus. The vector of the internuclear axis will be denoted by $\mathbf{R}$, while $\mathbf{r}_{12}$ represent the interelectron relative vector. Further, $\mathbf{r}_i(\mathbf{r}_f)$ is the position vector of the center of mass system $Z_T-e_1-e_2(Z_P-e_1-e_2)$ relative to $Z_P(Z_T)$, $\mathbf{K}_i$ and $\mathbf{K}_f$ are the initial and final momenta. The masses of projectile and target nucleus are M_P and M_T.

The 'prior' and the 'post' forms of the transition amplitude for process (2) in the first Born approximation with asymptotically correct boundary condition are the following:

$$\mathbf{T}_{if}^{(-)}(\mathbf{p})=\iiint d\mathbf{r}_i\, d\mathbf{r}_{P1}\, d\mathbf{r}_{P2}\, e^{i\mathbf{K}_f\mathbf{r}_f}\varphi_f^*(\mathbf{r}_{P1},\mathbf{r}_{P2}) \cdot\left[-\frac{\mathbf{Z}_P}{r_{P1}}-\frac{\mathbf{Z}_P}{r_{P2}}+\frac{2\mathbf{Z}_P}{\mathbf{R}}\right]e^{i\mathbf{K}_i\mathbf{r}_i}\varphi_i(\mathbf{r}_{T1},\mathbf{r}_{T2})\,E(R) \tag{3.a}$$

$$\mathbf{T}_{if}^{(+)}(\mathbf{p})=\iiint d\mathbf{r}_f\, d\mathbf{r}_{T1}\, d\mathbf{r}_{T2}\, e^{i\mathbf{K}_f\mathbf{r}_f}\varphi_f^*(\mathbf{r}_{P1},\mathbf{r}_{P2}) \cdot\left[-\frac{\mathbf{Z}_r}{r_{T1}}-\frac{\mathbf{Z}_T}{r_{T2}}+\frac{2\mathbf{Z}_T}{\mathbf{R}}\right]e^{i\mathbf{K}_i\mathbf{r}_i}\varphi_i(\mathbf{r}_{T1},\mathbf{r}_{T2})\,E(\mathbf{R}), \tag{3.b}$$

where,

$$E(\mathbf{R})=\exp\left\{i\frac{Z_P(Z_T-2)}{v}\ln(vR-\mathbf{vR}) +i\frac{Z_T(Z_P-2)}{v}\ln(vR+\mathbf{vR})\right\}, \tag{4}$$

$\varphi_f(\mathbf{r}_{P1},\mathbf{r}_{P2})$ and $\varphi_i(\mathbf{r}_{T1},\mathbf{r}_{T2})$ are the initial and final electronic wave functions, and $\mathbf{v}$ is the incident velocity vector. To order $O(1/M_P, 1/M_T)$ the term $\mathbf{K}_i\mathbf{r}_i+\mathbf{K}_f\mathbf{r}_f$ has a simple form $\mathbf{K}_i\mathbf{r}_i+\mathbf{K}_f\mathbf{r}_f=\mathbf{p}\mathbf{r}_i-\mathbf{v}\mathbf{r}_{P1}-\mathbf{v}\mathbf{r}_{P2}=-\mathbf{p}\mathbf{r}_f -\mathbf{v}\mathbf{r}_{T1}-\mathbf{v}\mathbf{r}_{T2}$, with $\mathbf{p}$ being the momentum transferred to the projectile (3a, b) shows that the electron-electron repulsion $1/r_{12}$ enters the problem through the unperturbed initial and final wave functions (static correlation) in this first order model. Higher order terms are required to include the dynamic correlation [12].

From now we concentrate on process (1), where most of the experimental and theoretical data are available. In this case the calculation is simplified because the logarithmic term $E(\mathbf{R})$ in (3a, b) vanishes. For describing the electronic ground state a configuration-interaction wave function of Joachim et al. [18] has been used:

$$\varphi^{CI}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{4\pi}\sum_{l=0}^{\lambda}\frac{4\pi}{2l+1}\sum_{m=-l}^{+l}F_1(\mathbf{r}_1,\mathbf{r}_2)$$

$$F_1(\mathbf{r}_1,\mathbf{r}_2)=\sum_{n\leqq k}\mathbf{A}_{n,k}^{(1)}(1+P_{1,2}^j)[\phi_{1+n,l,m}(\alpha,\mathbf{r}_1) \cdot\phi_{1+k,l,m}(\alpha,\mathbf{r}_2)] \tag{5}$$

with

$$\phi_{i,l,m}(\alpha,\mathbf{r})=r^i e^{\frac{-\alpha r}{2}}Y_{lm}(\hat{r}) \tag{6}$$

being the unnormalized Slater-type orbitals. Furthermore $n+k\leqq\mu$ and $\alpha=3.7$ is a nonlinear variational pa-

rameter. The coefficients $A_{n,k}^{(1)}$ are linear variational parameters whose values are obtained by the Rayleigh-Ritz method. $P_{1,2}^{j}$ $(j=i, f)$ is the operator which exchanges 1 and 2 and, Y_{lm} is the usual spherical harmonics. So the transition amplitude for the process (2) is a linear combination of the transition amplitudes ($f^{(+,-)}(\mathbf{p})$, see below) corresponding to each of the participating Slater orbitals

$$\mathbf{T}_{i,f}^{(+,-)}(\mathbf{p})=\sum_{l_i=0}^{\lambda_i}\sum_{l_f=0}^{\lambda_f}\sum_{m_i=-l_i}^{l_i}\sum_{m_f=-l_f}^{l_f}\sum_{n_i\leqq k_i}^{\mu_i}\sum_{n_f\leqq k_f}^{\mu_f}\mathbf{A}_{n_i k_i}^{l_i}\mathbf{A}_{n_f k_f}^{l_f}\cdot\frac{(1+P_{12}^{i})(1+P_{12}^{f})}{(2l_i+1)(2l_f+1)}f^{(+,-)}(\mathbf{p}) \tag{7}$$

where,

$$\mathbf{f}^{(-)}(\mathbf{p})=\iiint \mathrm{d}\mathbf{r}_i\,\mathrm{d}\mathbf{r}_{P1}\,\mathrm{d}\mathbf{r}_{P2}\,e^{iK_f\mathbf{r}_f}\phi_{l_f+n_f,l_f,m_f}^{*}(\mathbf{r}_{P1})\cdot\phi_{l_f+k_f,l_f,m_f}^{*}(\mathbf{r}_{P2})\left[-\frac{\mathbf{Z}_P}{r_{P1}}-\frac{\mathbf{Z}_P}{r_{P2}}+\frac{2\mathbf{Z}_P}{\mathbf{R}}\right]\cdot e^{iK_i\mathbf{r}_i}\phi_{l_i+n_i,l_i,m_i}(\mathbf{r}_{T1})\,\phi_{l_i+k_i,l_i,m_i}(\mathbf{r}_{T2}). \tag{8}$$

The subscripts i, f in (7, 8) label the initial and final quantities $\mathbf{f}^{(+)}(\mathbf{p})$ could be derived similarly (see (3 b)), so in the following we deal with the prior form of the transition matrix (3 a).

Introducing the Fourier transform and a partial wave representation of the wave function and the potentials, we get:

$$\mathbf{f}_{(nlm)_i}^{(-)}(\mathbf{p})=\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\cdots\sum_{l_7=0}^{\infty}\sum_{m_7=-l_7}^{l_7}\cdot\mathbf{D}_{lm}\,\mathbf{C}_{l_i0,l_20}^{l_i0}\,\mathbf{C}_{l_1m_1,l_2m_2}^{l_i-m_i}\,\mathbf{C}_{l_10,l_30}^{l_f0}\,\mathbf{C}_{l_1-m_1,l_3-m_3}^{l_fm_f}\cdot\mathbf{C}_{l_40,l_50}^{l_i0}\,\mathbf{C}_{l_4m_4,l_5m_5}^{l_im_i}\,\mathbf{C}_{l_40,l_60}^{l_f0}\,\mathbf{C}_{l_4m_4,l_6m_6}^{l_fm_f}\cdot\mathbf{C}_{l_60,l_70}^{l_30}\,\mathbf{C}_{l_6m_6,l_7m_7}^{l_3m_3}\cdot\mathbf{Y}_{l_2m_2}^{*}(\hat{\mathbf{v}})\,\mathbf{Y}_{l_5m_5}^{*}(\hat{\mathbf{v}})\,\mathbf{Y}_{l_7m_7}^{*}(\hat{\mathbf{p}})\,g_{l_il_fl_1+l_7}^{(-)}(p), \tag{9}$$

where,

$$\mathbf{D}_{lm}=(-i)^{l_1+l_6}i^{l_2+l_3+l_4+l_5+l_7}\cdot(-1)^{m_f+m_i}[l_i][l_f][l_1][l_3][l_4][l_6]([l_2][l_5][l_7])^{\frac{1}{2}},$$

$[l_k]=2l_k+1$, and $\mathbf{C}_{l_1m_1,l_2m_2}^{l_3m_3}$ is the Clebs-Gordan coefficient. Furthermore

$$\begin{aligned}g_{l_il_fl_1-l_7}^{(-)}(p)=(4\pi)^{\frac{3}{2}}&\int_0^{\infty}\mathrm{d}q_1\,q_1^2\cdot\left(E_1-\frac{q_1^2}{2}\right)G_{l_fn_f}(q_1)\,Q_{l_il_1l_2n_i}(q_1,v)\cdot\int_0^{\infty}\mathrm{d}q_2\,q_2^2\,G_{l_fk_f}(q_2)\,Q_{l_il_4l_5k_i}(q_2,v)\cdot S_{l_3l_6l_7}^{2}(p,q_1,q_2)\\&+(4\pi)^{\frac{3}{2}}\int_0^{\infty}\mathrm{d}q_1\,q_1^2\,G_{l_fn_f}(q_1)\,Q_{l_il_1l_2n_i}(q_1,v)\cdot\int_0^{\infty}\mathrm{d}q_2\,q_2^2\left(E_2-\frac{q_1^2}{2}\right)G_{l_fk_f}(q_2)\,Q_{l_il_4l_5k_i}(q_2,v)\cdot S_{l_3l_6l_7}^{2}(p,q_1,q_2)\\&+2Z_p(4\pi)^{\frac{3}{2}}\int_0^{\infty}\mathrm{d}q_1\,q_1^2\,G_{l_fn_f}(q_1)\,Q_{l_il_1l_2n_i}(q_1,v)\cdot\int_0^{\infty}\mathrm{d}q_2\,q_2^2\,G_{l_fk_f}(q_2)\,Q_{l_il_4l_5k_i}(q_2)\cdot S_{l_3l_6l_7}^{1}(p,q_1,q_2),\end{aligned} \tag{10}$$

with,

$$\begin{aligned}G_{li}(q)&=\int_0^{\infty}\mathrm{d}r\,r^{l+i+2}j_1(qr)\,e^{-\frac{\alpha}{2}}\\Q_{l_1l_2l_3n}(q,v)&=\int_0^{\infty}\mathrm{d}r\,r^{l_1+n+2}j_{l_2}(vr)j_{l_3}(qr)e^{-\frac{\alpha}{2}}\\S_{l_1l_2l_3}^{k}(p,q_1,q_2)&=\int_0^{\infty}\mathrm{d}r\,r^{k}j_{l_1}(pr)j_{l_2}(q_1r)j_{l_3}(q_2r),\end{aligned} \tag{11}$$

where $j_1(x)$ is the spherical Bessel function. E_j is the energy of the jth electron in the initial state ($E_0=E_1+E_2$) is the ground state energy of the He atom calculated with CI wave function, see (5)). Considering the above formulas the following remarks would be important regarding the physics involved. As the present description based on a first order model ($B1B$) the electrons interact separately with the distorted field $-Z_K/r_{Kk}+Z_K/R$ ($K=P, T$; $k=1, 2$, see (3)). The initial and final bound-state wave functions has a form of linear combinations of unnormalized Slater-type orbitals. As a consequence the transition amplitude is a linear combination of amplitudes described by (9, 10). Equation 10 describe the radial parts of the following processes. The first term characterize the product of the transition between appropriate Slater orbitals of the active (first) electron via the $-Z_K/r_{Kk}$ potential and an overlap between appropriate Slater orbitals (integration over q_1 and q_2, respectively, translation factors and other term are also involved). The different (initial and final) Slater orbitals are regarded as eigenfunctions of approximate (initial and final) Hamilton operators representing different parts of correlation and screening. So the nonvanishing overlap of these functions could also describe a real physical transition so it is retained also [12]. The other terms has a similar meanings. (It should also mention here that the orthogonality condition of the wave functions is a non necessary condition in the $B1B$ model [15].)

The cross section for a process specified in (1) is defined:

$$\sigma_{\mathrm{if}}=\frac{1}{2\pi v}\int_{p_{\min}}^{p_{\max}}|T_{\mathrm{if}}|^2\,p\,\mathrm{d}p, \tag{12}$$

where T_{if} is either $T_{\mathrm{if}}^{(+)}$ or $T_{\mathrm{if}}^{(-)}$ (because of the special feature of the process (1)), $p_{\min}=\Delta E/v$ and $p_{\max}=\infty$ are the minimum and maximum momentum transfers, and ΔE is the energy transfer during the collision. The three-dimensional integral, which is required to obtain the SDCS was performed using the Gauss-Legendre quadrature. In the case of rapidly oscillating integrals (see (11)) the ε-algorithm [19] was used to accelerate the computation. The summation in (9) was retained up to the $l_1-l_7\leqq 2$ values because of the large computing time. The estimated contribution of the additional terms were less than 5%.

Results and discussions

Single differential cross section for resonant double electron capture by alpha particle impinging on He($1s^2$) target calculated in the *B1B* approximation for moderately high energies is presented in Fig. 1. Two types of the correlated CI-wave functions corresponding to the number 12 and 60 of one-electron unnormalized Slater orbitals ($\mu=3$, 6 respectively, $n+k\leqq\mu$ see (5, 6)) were applied. The proper ground-state energy values are $E_0=-2.898$ a.u. and $E_0=-2.90227$, respectively. Differences between the total cross section data calculated with $\mu=3$ and $\mu=6$ parameters were less than 2%, which shows a very good convergence behavior of the CI wave function. (The curves in Figures correspond to the CI wave functions belonging parametrising the $\mu=3$). Uncorrelated bound state wave functions, i.e. a product of K-shell one electronic hydrogen-like orbitals with a variationally determined nuclear charge $Z=1.67$, and a product of $5-z$ HF Clementi-Roetti orbitals (RHF) [20] were also applied for comparison. At the lowest energies the SDCS values calculated with hydrogen-like functions are 10% higher than those calculated with CI wave functions. The difference slightly increases up to 25% (at 6 MeV) with increasing projectile energies. The tendency and the difference at lower energies is the same for RHF wave functions, however the deviations at the higher energy are larger (50% at 6 MeV). The increasing deviation with increasing impact energies in the SDCS values obtained with H-like and RHF functions is due to the difference between these orbitals at large momentum values.

The comparison of the *B1B* calculation using CI functions with experiments and theoretical approximations

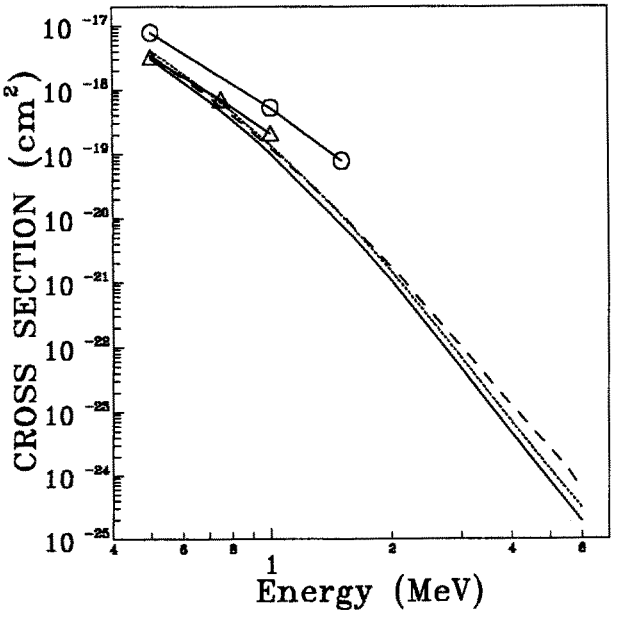
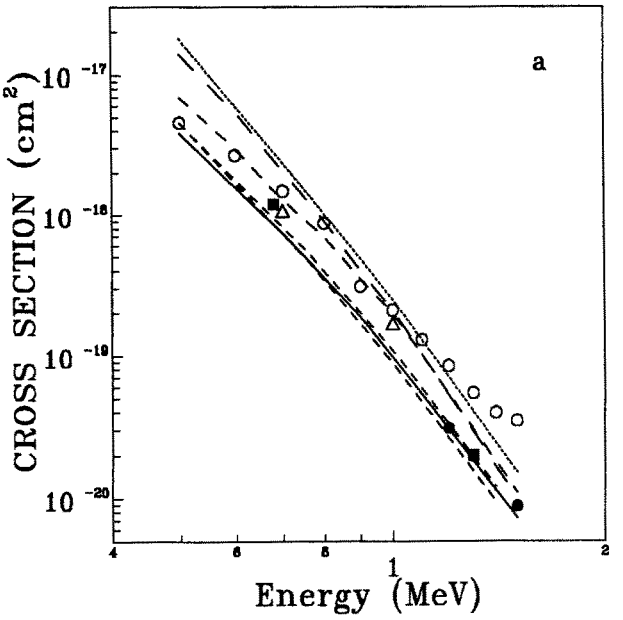


Fig. 1. Theoretical $1s^2-1s^2$ double-electron capture cross sections for $He^{2+}-He$ collision. Present *B1B* approximation applying the: CI, *solid line*; RHF, *dashed line*; H-like, *dotted line* wave functions. *Full line+circle*: first Born approach [8]; *full line+triangle*: two state atomic approach [9]



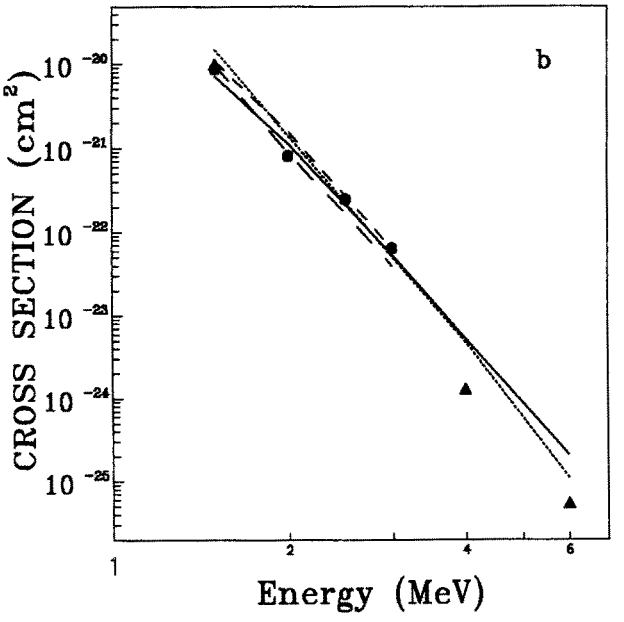


Fig. 2. **a** Total double capture cross sections for $He^{2+}-He$ collision. Theories are for the resonant collisions ($1s^2-1s^2$). *Solid line*: present *B1B* approach with CI wave function; *long dashed lines*: CDW approach [6]; *short dashed line*: CDW approach [11]; *dotted line*: CDW approach [13]; *dot-dashed line*: CDW-EIS approach [6]. Experiments for capture into all bound states: *open circles*: [2]; *full circles*: [5]; *open triangles*: [4]; *full triangles*: [7]; *open squares*: [3] *full squares*: [1]; **b** The same as Fig. 2a but for different impact energies

at different impact energy ranges 0.5–1.5 MeV and 1.5–6.0 MeV is given in Fig. 2a, b, respectively. It is seen that the energy dependence of the experimental results from [1, 5, 7] is in agreement with the predictions of different theories. There are deviations among the SDCS values predicted by the calculations using different types of wave functions, especially in the lower energy range where most of the data are available. (Here it is impor-

tant to note the limited validity some of these theories). In the case of the independent particle approximation a very good agreement with the experimental data is found with the CDW-EIS calculation in the whole energy region, while the CDW one predicts higher values at the lowest energies [17]. The tendency is the same in these two models in describing the single capture processes. Differences are also found between the CDW calculations using different types of correlated wave functions especially at lower impact energies. (In [6] and [13] the same CDW code were used and in [11] the sequence of events was allowed.) The present *B1B* approximation using CI wave function is in good agreement with the experimental data especially in the higher impact energy region where the model is applicable for the single electron capture. This implies that the double or multiple scattering phenomena, described by higher order theories does not influence essentially the double capture process (1) in the above energy region. However relating to this conclusion the deviations among the experimental data should also mentioned.

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Note added in proof. After submitting the present manuscript, the authors became aware of another calculation of the double capture within a CB1 approximation (Belkic, Dž.: Phys. Rev. A **47**, 189 (1993)) resulting in a higher cross section. The source of this discrepancy has not found yet.

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